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6. AUTHOR(S)
Professor John Maddocks

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Dept of Mathematics
University of Maryland
College Park, MD 20742

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13. ABSTRACT *(Maximum 200 words)*

The general objective of this research program is the development and application of new methods of analysis, numerical analysis, scientific computation visualization techniques within the context of specific nonlinear mechanics problems that model significant physical phenomena. In general mathematical terms the analysis and numerics can be classified as dealing with problems of continuation, bifurcation, and stability exchange as they arise in the variational principles of mechanics, and especially within the context of Hamiltonian systems. The fields of application all have these themes as common mathematical underpinnings, but specific models are as diverse as describing gravity-gradient effects on the attitude dynamics of large satellites, or the supercoiling and molecular dynamics of long-chain macro-molecules such as DNA. The guiding philosophy of the research is that substantial progress can be made by simultaneously considering context-specific modeling issues along with the development of new and generally applicable analytical and numerical techniques. Within the project there is a particular emphasis on the exploitation of computation combined with interactive visualization to provide understanding of data, and to generate insight and conjectures that lead to analytical conclusions.

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Final Report

John H. Maddocks,
Institute for Physical Science and Technology,
and Department of Mathematics,
University of Maryland,
College Park MD 20742
jhm@sonya.umd.edu, (301) 405 7641

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The general objective of this research program is the development and application of new methods of analysis, numerical analysis, scientific computation and visualization techniques, within the context of specific nonlinear mechanics problems that model significant physical phenomena. In general mathematical terms the analysis and numerics can be classified as dealing with problems of continuation, bifurcation, and stability exchange as they arise in the variational principles of mechanics, and especially within the context of Hamiltonian systems. The fields of application all have these themes as common mathematical underpinnings, but the specific models are as diverse as describing gravity-gradient effects on the attitude dynamics of large satellites, or the supercoiling and molecular dynamics of long-chain macro-molecules such as DNA. The guiding philosophy of the research is that substantial progress can be made by simultaneously considering context-specific modelling issues along with the development of new and generally applicable analytical and numerical techniques. Within the project there is a particular emphasis on the exploitation of computation combined with interactive visualization to provide understanding of data, and to generate insight and conjectures that lead to analytical conclusions.

In the past year progress has been made in the following areas:

A: Analysis Many systems can naturally be formulated as Lagrangian systems that are subject to constraints. Consideration of the dynamics of inextensible and unshearable rods (reference [5] below) led to a novel *unconstrained* Hamiltonian formulation of a rather general class of such Lagrangian systems. The desired constraint is by construction a first integral of the Hamiltonian dynamics. However the Hamiltonian, $H(x,y)$ say, is only defined after an auxiliary minimization

$$H(x,y) = \min_{\Lambda} \tilde{H}(x,y,\Lambda),$$

where we call $\tilde{H}(x,y,\Lambda)$ the *pre-Hamiltonian*. Here y is the variable conjugate to the configuration variable x, but in applications y is typically not the classic momentum or impulse, and so we give it a new name, the *impetus*. In applications the quantity Λ is generally the time anti-derivative of a familiar physical quantity, e.g. for incompressible fluid flow (reference [6]) Λ_t is the pressure field. Λ can also be interpreted as a Lagrange multiplier enforcing a time-differentiated constraint, but to distinguish it from the usual multiplier, we call Λ the *striction*. In the context of systems of ordinary differential equations the impetus-striction formulation can be viewed as a variant of the vakonomic mechanics of Kozlov, but the impetus-striction description naturally extends to systems of partial differential equations. The new formulation has already proven effective in obtaining analytical stability results [5]. This work comprises a large part of the PhD research of D. Dichmann who recently successfully defended his thesis. Dichmann is one of the students supported under the AASERT supplement to this project. Numerical methods based on the impetus-striction approach are currently under investigation.

The second analytical development concerns the effects of dissipation on the characterization of stability properties in Hamiltonian systems (Article [7] below). The result is most simply stated in the case of equilibria of ordinary differential equations. Consider the perturbed (autonomous, canonical) Hamiltonian system

$$\dot{z} = (J - \epsilon D)\nabla H(z),$$

with J skew and nonsingular, and D symmetric and positive semi-definite. Then the equilibria z_e of the dynamics are precisely the critical points of the Hamiltonian. For $\epsilon \geq 0$ it is easy to see that minima of the Hamiltonian are necessarily dynamically stable, and it is also known that in the case $\epsilon = 0$ non-minima can also be dynamically stable (in the full nonlinear sense). The new result states that for $\epsilon > 0$ and for a natural class of dissipations D (including classic Rayleigh dissipation), the number of unstable modes of the linearized dynamics coincides with the index of z_e regarded as a critical point of H. Special cases of this result trace back to Kelvin, and are also of contemporary concern, but the generality of this result, with no assumption on simplicity of eigenvalues for example, is new. The result is significant because it allows effects of dissipation on dynamic stability to be analyzed from a purely static, variational viewpoint. The proof is a simple continuation argument that can also be applied in the context of various Hamiltonian partial differential equations.

B: Applications areas Two areas of application have been of primary concern. The first concerns non-canonical Hamiltonian systems and gravity-gradient effects on the attitude dynamics of satellites. In an extension of completed but somewhat qualitative work, and now in collaboration with Captain C. D. Hall of the Aerospace Engineering Department at the Air Force Institute of Technology (who is supervising a Ph.D. thesis on this topic) we are undertaking a quantitative investigation of whether the standard approximate model used for predicting steady-state attitudes of satellites can give incorrect answers in parameter regimes that arise for existing and envisioned satellite missions. The analytical and numerical projects concerning the dynamics of rods and effects of dissipative perturbations also pertain to this area of application because of issues arising with the motion of long aerials and tether systems.

The second area of application is the supercoiling of long chain molecules such as DNA. In the context of DNA the local atomic structure is known to be the classic double helix. The point of interest is how the double helix itself deforms and coils around itself or other objects such as proteins. This problem is of considerable contemporary interest to molecular biologists, chemists and mathematicians with a background in topology and knot theory (witness the IMA 1994 Summer Program in Topological Issues in DNA). However the heart of the problem lies in issues of mechanics. Over the past year with a postdoc Y. Li we have developed a model for the equilibrium supercoiling of DNA both with and without effects of self-contact. From the outset the model has been developed to be amenable to efficient computation, but the formulation we use has also provided several analytical insights. By using modern theories of rod mechanics combined with the impetus-striction formulation mentioned above, the model is reduced to a two-point boundary value problem for a seven degree of freedom Hamiltonian system. In the case of self-contact three of the "ordinary" differential equations involve nonlocal terms expressed in terms of quadratures. In either case the problem can be efficiently discretized by the collocation method, and we have been using a solver and path following algorithms that are adaptations of the package AUTO.

In addition to applications in modelling DNA, the work applies equally well to other long chain molecules. For example tropomyosin is a large "coiled-coiled" molecule comprised of two alpha helices interwound with each other, and the overall molecular structure is of considerable interest to biochemists. Similar systems arise in many other large molecules that are of interest to the Air Force. One application is that such coiled-coiled molecules have considerable potential for use as substrates to make materials that are optically highly nonlinear. Joint investigations

with Dr. Ruth Pachter of the Laser Hardening Division at the Wright Paterson Materials Science Laboratory are pursuing this line of investigation. At a completely different scale the same code can be used to model highly twisted and contorted wires that arise in cross-disciplinary applications such as intravenous surgical techniques using guidewires, or the construction of deployable space structures or aerials with complicated, possibly knotted, geometries.

C: Numerical Algorithms In joint work with a postdoc J.-M. Xu we have constructed conservative algorithms for the numerical integration of (autonomous) Hamiltonian systems of ordinary differential equations. The algorithms have the property that they exactly (to machine precision) conserve the Hamiltonian (if autonomous) and also all other known integrals of the continuous system. The main idea is to enforce a compatability condition between the choice of time step and the discretization of the gradient operator, in order to construct a discrete chain rule. This discrete chain rule automatically implies conservation of the Hamiltonian, and conservation of the other invariants can be guaranteed by a rather natural and simple projection technique that only involves the solution of a (small) linear system. So far a simple second-order scheme has been implemented and tested on various classic Hamiltonian systems, such as the Kepler problem. The results are extremely competitive with both general purpose, and symplectic integrators. Higher order, stable, multi-step methods such as Gear's BDF schemes can also be modified to be made conservative, but the resulting schemes are quite expensive in terms of function evaluations, and it is as yet unclear whether the increase in order results in a corresponding increase in efficiency.

The most obvious motivation to construct conservative schemes for Hamiltonian systems is a natural desire to conserve physical quantities such as energy and angular momentum. However numerical implementations based upon the impetus-striction formulation of constrained Lagrangian systems as unconstrained Hamiltonian systems provides another compelling motivation. In such systems the constraints are by construction integrals of the (continuous) Hamiltonian system, and so it is desirable that they be preserved by the numerical algorithm in order for the system to make sense.

D: Scientific Computation and Visualization The group is involved in a number of projects exploiting advanced visualization techniques combined with interactive computation in parameter dependent problems. Much of this work is done by calling customized computational code from within the commercial graphics package AVS. For development purposes practically all of the computation is run on a small local cluster of DEC alpha workstations with Kubota graphics accelerators on two machines. However some calculations are carried out remotely on the San Diego Cray, and on the University of Maryland CM5. Working within the AVS package vastly decreases the required graphics programming time, and allows effort to be concentrated on the scientific and numerical issues. One project is the continued development of the package MC^2 (Multiplier and Constraint Continuation) which allows interactive exploration of the set of critical points of two-parameter variational principles, with simultaneous display of various projections of the bifurcation surface, and determination of stability properties. The current version of MC^2 is particularly optimized to explore the sets of equilibria and relative equilibria of Hamiltonian systems of ordinary differential equations as arise, for example, in the steady-spins of satellites affected by external fields. In the past year, progress has been made toward extension to analogous systems of partial differential equations in time and one space dimension. Then the problem to be treated by MC^2 is a two-point boundary value problem for a nonlinear system of ordinary differential equations governing steady-state solutions. For such systems a very natural data compression is immediately available. Once the two-point boundary value problem has been solved, by parameter continuation methods combined with collocation or whatever other approach is desired, the only data that need be stored are an appropriate set of initial conditions for each parameter value. All

other data can be easily, and essentially instantaneously, recovered by running an appropriate initial value-problem solver. The package PCR (developed by Domokos and Paffenroth) exploits this idea to provide a graphics based tool for understanding bifurcation problems. Two graphics windows are provided, one displays four scalars along the (locally) one-dimensional families of solutions using three dimensional coordinates plus a color scale. Points on these curves can be selected by a single mouse-click, which causes the appropriate initial data to be sent to the initial value problem solver, and an appropriate projection of the actual solution for that parameter value is displayed in a second window. The tool is designed for general use, but has been developed and used extensively in the specific context of the DNA modelling problem described above. There the graphical display of the solution allows the knot type, and contact regions to be easily understood, and the graphical connection between points in the bifurcation diagram and the corresponding solution lays bare the (quite complicated) symmetry relations between solutions on different branches. Paffenroth, who is a student of Maddocks, is in only his second year of graduate study. For the current year he is assuming the final year of the AASERT award that has been freed up by the graduation of Dichmann. An application for another AASERT award will be made to continue the support of Paffenroth.

E: External Collaborations

Contacts with various government and industrial research laboratories are steadily increasing. In a project jointly funded by the Industrial Mathematics Postdoctoral Program of the Division of Mathematical Sciences at the NSF and by Computer Sciences Corporation, Dichmann (who just successfully defended his thesis, and was supported under the above mentioned AASERT award) will be working on Hamiltonian models of the attitude dyanmics of artificial satellites. The idea is to consider the implications of some of my groups recent work in Hamiltonian systems within the context of actual satellite missions. In particular we plan to use real satellite design parameters in computations based on the Hamiltonian models and to compare the results both with actual flight data, and with the output of models that are currently used in mission design. For example it is planned to consider a combination of the analyses in [1] and [4] above as a model for the extremely long and flexible antennas that are present in many contemporary satellites. The work will also consider prior work of mine concerning Hamiltonian models of gravity-gradient attitude dynamics within the context of quantitative comparison with real satellite data. The division of Computer Sciences Corporation that is involved in funding this work is associated with NASA so Dichmann will be primarily using NASA data. However the project also involves continuation of an ongoing collaboration between myself and Professor C.A. Hall of the Air Force Institute of Technology and his students. Hall has recently established contact with the NRL to obtain Navy satellite data for comparison with computations based on my gravity-gradient model. Consequently I will also certainly investigate the possibility of closer direct contact between my group and interested parties at the NRL.

The computations of myself and Li concerning rods have also led to non-academic collaborations. The application as a model for DNA supercoiling led to contact with Dr. Ruth Pachter of the Laser Hardened Materials Division of the Materials Laboratory at Wright Patterson Air Force Base. They are interested in various long chain coiled-coil molecules both for their nonlinear optical response and their extremely strong material properties (Kevlar is of this form for example). With Pachter I am planning an extensive program in computation and models of molecular mechanics.

The recent conference run by Pachter at WPAFB also lead to a potentially useful contact with Moldyn Inc which is a small Massachussets company that is concerned with the development of molecular dynamics codes. They are a spin-off of another company that is concerned with the maintenance and development of a multi-rigid body dynamics code called DISCOS for NASA Goddard. A three way meeting with Pachter, Moldyn and myself is currently being planned for

later this fall with the objective of investigating whether the impetus-striction ideas described above might be of interest in the code development activities of Moldyn and its parent company in the areas of both molecular dynamics and spacecraft dynamics.

My computations with rods also led to contact with Dr. Brian Berg of Fleximedics Corporation, Minnesota. They manufacture various medical devices with wire made out of NITINOL (the shape memory alloy developed largely by the Navy). For their purposes the reversible austenite-martensite phase transition exhibited by NITINOL allows them to manufacture wires whose unstressed states are of any desired form and which are highly elastic, i.e. they can suffer large strain deformations without undergoing plastic deformation. However in some applications some samples exhibit highly nonlinear responses to twist loading, which is a very undesirable feature. My Hamiltonian model of rod statics (as described above) predicts that such effects would be present in rods that had manufacturing imperfections which perturbed the relations between material and rigid-body symmetries. We are presently entering a program of computation and experiment to see whether this qualitative explanation can indeed give quantitative predictions and ultimately a simple to test to reject undesirable samples.

Articles Appeared, Accepted or Submitted in Last Year

1. (with J.C. Alexander) "Bounds on the friction-dominated motion of a pushed object", Int. J. Robotics Research, **12** #3 (1993) pp. 231–248
2. (with R.L. Sachs) "On the stability of KdV multi-solitons", Comm. Pure and Applied Math. **46** (1993) pp. 867–901
3. (with D.J. Dichmann) "Conservation laws in the dynamics of rods", J. Elasticity **34** (1994) pp. 83–96
4. (with R. Nair) "On the forward kinematics of parallel manipulators", Int. J. Robotics Research, **13** #2 (1994) pp. 171–188
5. (with D.J. Dichmann and R.L. Pego) "Hamiltonian dynamics of an elastica and the stability of solitary waves", Arch. Rat. Mech. Anal. (37 pages) accepted
6. (with R.L. Pego) "An unconstrained Hamiltonian formulation for incompressible fluid flow" (14 pages) Comm. Math. Physics, accepted
7. (with M.L. Overton) "Stability Theory for Dissipatively Perturbed Hamiltonian Systems" (26 pages) Comm. Pure Applied Math, submitted
8. (with R.L. Sachs) "Constrained Variational Principles and Stability in Hamiltonian Systems", to appear in "*Hamiltonian Dynamical Systems*", *IMA Volumes in Mathematics and Its Applications*, Eds. S. Dumas , K. Meyer and D. Schmidt. (30 pages) (to appear 1994)
9. (by R. C. Paffenroth and G. Domokos) "PCR-A Visualization Tool for Multi-Point Boundary Value Problems" Institute for Physical Science and Technology, Technical Report, BN-1167, (1994)